Deep Directed Generative Autoencoders

Sherjil Ozair
Indian Institute of Technology Delhi

Yoshua Bengio
Université de Montréal
CIFAR Fellow

Abstract

For discrete data, the likelihood $P(x)$ can be rewritten exactly and parametrized into $P(X = x) = P(X = x|H = f(x))P(H = f(x))$ if $P(X|H)$ has enough capacity to put no probability mass on any x' for which $f(x') \neq f(x)$, where $f(\cdot)$ is a deterministic discrete function. The log of the first factor gives rise to the log-likelihood reconstruction error of an autoencoder with $f(\cdot)$ as the encoder and $P(X|H)$ as the (probabilistic) decoder. The log of the second term can be seen as a regularizer on the encoded activations $h = f(x)$, e.g., as in sparse autoencoders. Both encoder and decoder can be represented by a deep neural network and trained to maximize the average of the optimal log-likelihood $\log p(x)$. The objective is to learn an encoder $f(\cdot)$ that maps X to $f(X)$ that has a much simpler distribution than X itself, estimated by $P(H)$. This "flattens the manifold" or concentrates probability mass in a smaller number of (relevant) dimensions over which the distribution factorizes. Generating samples from the model is straightforward using ancestral sampling. One challenge is that regular back-propagation cannot be used to obtain the gradient on the parameters of the encoder, but we find that using the straight-through estimator works well here. We also find that although optimizing a single level of such architecture may be difficult, much better results can be obtained by pre-training and stacking them, gradually transforming the data distribution into one that is more easily captured by a simple parametric model.

1 Introduction

Deep learning is an aspect of machine learning that regards the question of learning multiple levels of representation, associated with different levels of abstraction (Bengio, 2009). These representations are distributed (Hinton, 1989), meaning that at each level there are many variables or features, which together can take a very large number of configurations.

An important conceptual challenge of deep learning is the following question: *what is a good representation*? The question is most challenging in the unsupervised learning setup. Whereas we understand that features of an input x that are predictive of some target y constitute a good representation in a supervised learning setting, the question is less obvious for unsupervised learning.

1.1 Manifold Unfolding

In this paper we explore this question by following the geometrical inspiration introduced by Bengio (2014), based on the notion of *manifold unfolding*, illustrated in Figure 2. It was already observed by Bengio *et al.* (2013a) that representations obtained by stacking denoising autoencoders or RBMs appear to yield "flatter" or "unfolded" manifolds: if x_1 and x_2 are examples from the data generating distribution $Q(X)$ and f is the encoding function and g the decoding function, then points on the line $h_\alpha = \alpha f(x_1) + (1-\alpha)f(x_2)$ ($\alpha \in [0, 1]$) were experimentally found to correspond to probable input configurations, i.e., $g(h_\alpha)$ looks like training examples (and quantitatively often comes close to one). This property is not at all observed for f and g being the identity function: interpolating in input space typically gives rise to non-natural looking inputs (we can immediately recognize such inputs as the simple addition of two plausible examples). This is illustrated in Figure 1. It means that the input manifold (near which the distribution concentrates) is highly twisted and curved and occupies a small volume in input space. Instead, when mapped in the representation space of stacked autoencoders (the output of f), we find that the convex between high probability points (i.e., training examples) is often also part of the high-probability manifold, i.e., the transformed manifold is flatter, it has become closer to a convex set.

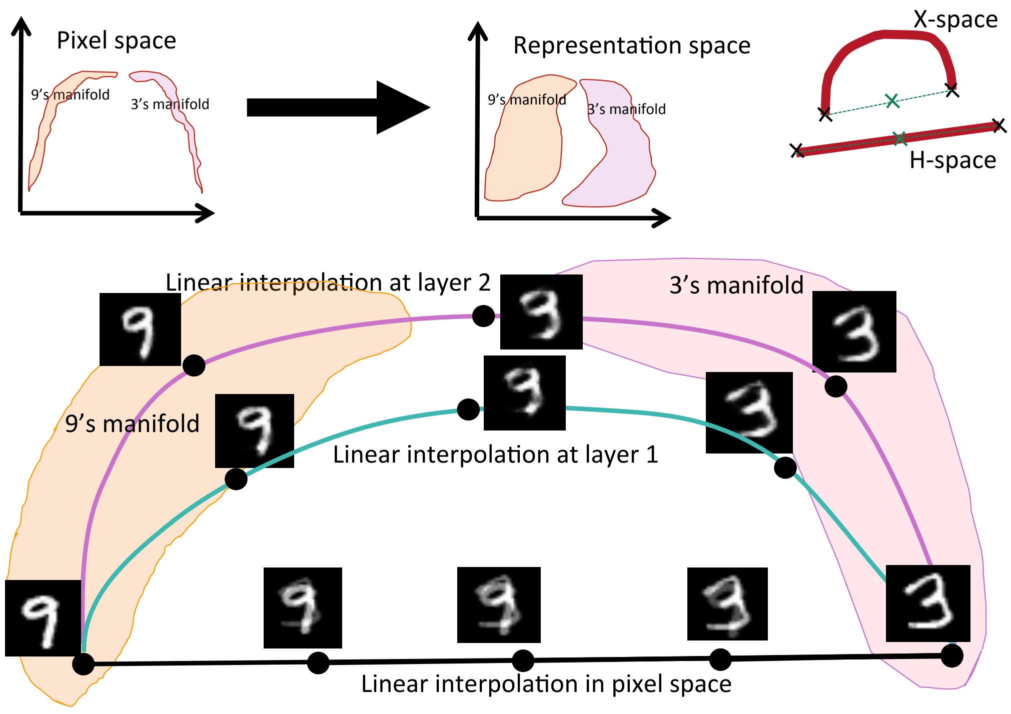

Figure 1: Illustration of the flattening effect observed in Bengio *et al.* (2013a) by stacks of denoising autoencoders or RBMs, trained on MNIST digit images. Whereas interpolating in pixel space (X-space) between dataset examples (such as the 9 on the bottom left and the 3 on the bottom right) gives rise to images unlike those in the training set (on the bottom interpolation line), interpolating at the first and second level of the stack of autoencoders (H-space) gives rise to images (when projected back in input space, see text) that look like dataset examples. These experiments suggest that the manifolds near which data concentrate, which are very twisted and occupy a very small volume in pixel space, become flatter and occupy more of the available volume in representation-space. Note in particular how the two class manifolds have been brought closer to each other (but interestingly there are also easier to separate, in representation space). The manifolds associated with each class have become closer to a convex set, i.e., flatter.

1.2 From Manifold Unfolding to Probability Modeling

If it is possible to unfold the data manifold into a nearly flat and convex manifold (or set of manifolds), then estimating the probability distribution of the data becomes much easier. Consider the situation illustrated in Figure 2: a highly curved 1-dimensional low-dimensional manifold is unfolded so that it occupies exactly one dimension in the transformed representation (the "signal dimension" in the figure). Moving on the manifold corresponds to changing the hidden unit corresponding to that signal dimension in representation space. On the other hand, moving orthogonal to the manifold in input space corresponds to changing the "noise dimension". There is a value of the noise dimension that corresponds to being on the manifold, while the other values correspond to the volume filled by unlikely input configurations. With the manifold learning mental picture, estimating the probability distribution of the data basically amounts to distinguishing between "off-manifold" configurations, which should have low probability, from "on-manifold" configurations, which should have high probability. Once the manifold is unfolded, answering that question becomes very easy.

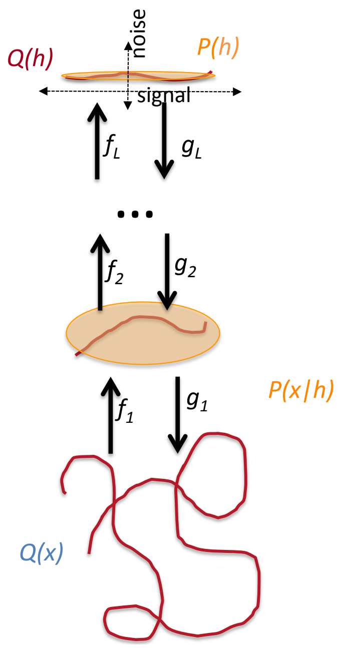

Figure 2: Illustration of the work that the composed encoder $f = f_L \circ \ldots f_2 \ldots f_1$ should do: flatten the manifold (more generally the region where probability mass is concentrated) in such a way that a simple (e.g. factorized) prior distribution $P(h)$ can well approximate the distribution of the transformed data $Q(h)$ obtained by applying f to the data $x \sim Q(x)$. The red curve indicates the manifold, or region near which $Q(x)$ concentrates. The first encoder f_1 is not powerful and non-linear enough to untwist the manifold and flatten it, so applying a factorized prior at that level would yield poor samples, because most generated samples from the prior (in orange) would fall far from the transformed data manifold (in red). At the top level, if training is successful, the transformed data distribution $Q(h)$ concentrates in a small number of directions (the "signal" directions, in the figure), making it easy to distinguish the inside of the manifold (signal) from the outside (noise), i.e. to concentrate probability mass in the right places. At that point, $Q(h)$ and $P(h)$ can match better, and less probability mass is wasted outside of the manifold.

If probability mass is concentrated in a predictible and regular way in representation space (H), it becomes easy to capture the data distribution $Q(X)$. Let $H = f(X)$ be the random variable associated with the transformed data $X \sim Q(X)$, with $Q(H)$ its marginal distribution. Now, consider for example the extreme case where $Q(H)$ is almost factorized and can be well approximated by a factorized distribution model $P(H)$. It means that the probability distribution in H-space can be captured with few parameters and generalization is easy. Instead, when modeling data in X-space, it is very difficult to find a family of probability distributions that will put mass where the examples are but not elsewhere. What typically happens is that we end up choosing parameters of our probability model such that it puts a lot more probability mass outside of the manifold than we would like. The probability function is thus "smeared". We clearly get that effect with non-parametric kernel density estimation, where we see that the kernel bandwidth controls the amount of smearing, or smoothing. Unfortunately, in a high-dimensional space, this puts a lot more probability mass outside of the manifold than inside. Hence what we see the real challenge as finding an encoder f that transforms the data distribution $Q(X)$ from a complex and twisted one into a flat one, $Q(H)$, where the elements H_i of H are easy to model, e.g. they are independent.

2 Directed Generative Autoencoder (DGA) for Discrete Data

We mainly consider in this paper the case of a discrete variable, which is simpler to handle. In that case, a Directed Generative Autoencoder (DGA) is a model over the random variable X whose training criterion is as follows

$$\log P(X = x|H = f(x)) + \log P(H = f(X)) \tag{1}$$

where the deterministic function $f(\cdot)$ is called the encoder and the conditional distribution $P(x|h)$ is called the decoder or decoding distribution. As shown below (Proposition 1), this decomposition becomes exact as the capacity of the decoder $P(x|h)$ increases sufficiently to capture a conditional distribution that puts zero probability on any x' for which $f(x') \neq h$. The DGA is parametrized from two components:

1. $P(X = x|H = f(x))$ is an autoencoder with a *discrete* representation $h = f(x)$. Its role in the log-likelihood training objective is to make sure that f preserves as much information about x as possible.
2. $P(H = h)$ is a probability model of the samples $H = f(X)$ obtained by sending X through f. Its role in the log-likelihood training objective is to make sure that f transforms X in a representation that has a distribution that can be well modeled by the family of distributions $P(H)$.

What can we say about this training criterion?

Proposition 1. *There exists a decomposition of the likelihood into $P(X = x) = P(X = x|H = f(x))P(H = f(X))$ that is exact for discrete X and H, and it is achieved when $P(x|h)$ is zero unless $h = f(x)$. When $P(x|h)$ is trained with pairs $(X = x, H = f(x))$, it estimates and converges (with enough capacity) to a conditional probability distribution which satisfies this contraint. When $P(x|h)$ does not satisfy the condition, then the unnormalized estimator $P^*(X = x) = P(X = x|H = f(x))P(H = f(X))$ underestimates the true probability $P(X = x) = \sum_h P(x|H = h)P(H = h)$.*

Proof. We start by observing that because $f(\cdot)$ is deterministic, its value $f(x)$ is perfectly predictible from the knowledge of x, i.e.,

$$P(H = f(x)|X = x) = 1. \tag{2}$$

Therefore, we can multiply this value of 1 by $P(X)$ and obtain the joint $P(X, H)$:

$$P(X = x) = P(H = f(x)|X = x)P(X = x) = P(X = x, H = f(x)) \tag{3}$$

for any value of x. Now it means that there exists a parametrization of the joint $P(X, H)$ into $P(H)P(X|H)$ that achieves

$$P(X = x) = P(X = x|H = f(X))P(H = f(X)) \tag{4}$$

which is the first part of the claimed result. Furthermore, for exact relationship with the likelihood is achieved when $P(x|h) = 0$ unless $h = f(x)$, since with that condition,

$$P(X = x) = \sum_h P(X = x|H = h)P(H = h) = P(X = x|H = f(x))P(H = f(x))$$

because all the other terms of the sum vanish. Now, consider the case (which is true for the DGA criterion) where the parameters of $P(x|h)$ are only estimated to maximize the expected value of the conditional likelihood $\log P(X = x|H = f(x))$. Because the maximum likelihood estimator is consistent, if the family of distributions used to estimate $P(x|h)$ has enough capacity to contain a solution for which the condition of $P(x|h) = 0$ for $h \neq f(x)$ is satisfied, then we can see that with enough capacity (which may also mean enough training time), $P(x|h)$ converges to a solution that satisfies the condition, i.e., for which $P(x) = P(x|H = f(x))P(H = f(x))$. In general, a learned decoder $P(x|h)$ will not achieve the guarantee that $P(x|h) = 0$ when $h \neq f(x)$. However, the correct $P(x)$, for given $P(x|h)$ and $P(h)$ can always be written

$$P(x) = \sum_h P(x|h)P(h) \geq P(x|h = f(x))P(H = f(x)) = P^*(x)$$

which proves the claim that $P^*(x)$ underestimates the true likelihood. □

What is particularly interesting about this bound is that *as training progresses and capacity increases* the bound becomes tight. However, if $P(x|h)$ is a parametric distribution (e.g. factorized Binomial, in our experiments) whose parameters (e.g. the Binomial probabilities) are the output of a neural net, increasing the capacity of the neural net may not be sufficient to obtain a $P(x|h)$ that satisfies the desired condition and makes the bound tight. However, if $f(x)$ does not lose information about x, then $P(x|f(x))$ should be unimodal and in fact be just 1. In other words, we should penalize the reconstruction error term strongly enough to make the reconstruction error nearly zero. That will guarantee that $f(x)$ keeps all the information about x (at least for x in the training set) and that the optimal $P(x|h)$ fits our parametric family.

2.1 Parameters and Training

The training objective is thus a lower bound on the true log-likelihood:

$$\log P(x) \geq \log P^*(x) = \log P(x|H = f(x)) + \log P(H = f(x)) \tag{5}$$

which can be seen to have three kinds of parameters:

1. The encoder parameters associated with f.
2. The decoder parameters associated with $P(x|h)$.
3. The prior parameters associated with $P(h)$.

Let us consider how these three sets of parameters could be optimized with respect to the log-likelihood bound (Eq. 5). The parameters of $P(h)$ can be learned by maximum likelihood (or any proxy for it), with training examples that are the $h = f(x)$ when $x \sim Q(X)$ is from the given dataset. For example, if $P(H)$ is a factorized Binomial, then the parameters are the probabilities $p_i = P(H_i = 1)$ which can be learned by simple frequency counting of these events. The parameters for $P(x|h)$ can be learned by maximizing the conditional likelihood, like any neural network with a probabilistic output. For example, if $X|H$ is a factorized Binomial, then we just have a regular neural network taking $h = f(x)$ as input and x as target, with the cross-entropy loss function.

2.2 Gradient Estimator for f

One challenge is to deal with the training of the parameters of the encoder f, because f is discrete. We need to estimate a gradient on these parameters in order to both optimize f with respect to $\log P(h = f(x))$ (we want f to produce outputs that can easily be modeled by the family of distributions $P(H)$) and with respect to $\log P(x|h = f(x))$ (we want f to keep all the information about x, so as to be able to reconstruct x from $h = f(x)$). Although the true gradient is zero, we need to obtain an update direction (a pseudo-gradient) to optimize the parameters of the encoder with respect to these two costs. A similar question was raised in a different context in Bengio (2013); Bengio *et al.* (2013b), and a number of possible update directions were compared. In our experiments we considered the special case where

$$f_i(x) = 1_{a_i(x)>0}$$

where a_i is the activation of the i-th output unit of the encoder before the discretizing non-linearity is applied. The actual encoder output is discretized, but we are interested in obtaining a "pseudo-gradient" for a_i, which we will back-propagate inside the encoder to update the encoder parameters. What we did in the experiments is to compute the derivative of the reconstruction loss and prior loss

$$\mathcal{L} = -\log P(x|h = f(x)) - \log P(h = f(x)), \tag{6}$$

with respect to $f(x)$, as if $f(x)$ had been continuous-valued. We then used the **Straight-Through Pseudo-Gradient**: the update direction (or pseudo-gradient) for a is just set to be equal to the gradient with respect to $f(x)$:

$$\Delta a = \frac{\partial \mathcal{L}}{\partial f(x)}.$$

The idea for this technique was proposed by Hinton (2012) and was used very succesfully in Bengio *et al.* (2013b). It clearly has the right sign (per value of $a_i(x)$, but not necessarily overall) but does not take into account the magnitude of $a_i(x)$ explicitly.

Let us see how the prior negative log-likelihood bound can be written as a function of $f(x)$ in which we can pretend that $f(x)$ is continuous. For example, if $P(H)$ is a factorized Binomial, we write this negative log-likelihood as the usual cross-entropy:

$$-\sum_i f_i(x)\log P(h_i=1)+(1-f_i(x))\log(1-P(h_i=1))$$

so that if $P(x|h)$ is also a factorized Binomial, the overall loss is

$$\begin{aligned}\mathcal{L}=&-\sum_i f_i(x)\log P(h_i=1)+(1-f_i(x))\log(1-P(h_i=1))\\&-\sum_j x_j\log P(x_j=1|h=f(x))+(1-x_j)\log(1-P(x_j=1|h=f(x)))\end{aligned} \quad (7)$$

and we can compute $\frac{\partial\mathcal{L}}{\partial f_i(x)}$ as if $f_i(x)$ had been a continuous-valued variable. All this is summarized in Algorithm 1.

Algorithm 1 Training procedure for Directed Generative Autoencoder (DGA).

```
• Sample $x$ from training set.
• Encode it via feedforward network $a(x)$ and $h_i = f_i(x) = 1_{a_i(x)>0}$.
• Update $P(h)$ with respect to training example $h$.
• Decode via decoder network estimating $P(x|h)$.
• Compute (and average) loss $\mathcal{L}$, as per Eq. 6, e.g., in the case of factorized Binomials as per Eq. 7.
• Update decoder in direction of gradient of $-\log P(x|h)$ w.r.t. the decoder parameters.
• Compute gradient $\frac{\partial\mathcal{L}}{\partial f(x)}$ as if $f(x)$ had been continuous.
• Compute pseudo-gradient w.r.t. $a$ as $\Delta a = \frac{\partial\mathcal{L}}{\partial f(x)}$.
• Back-propagate the above pseudo-gradients (as if they were true gradients of the loss on $a(x)$) inside encoder and update encoder parameters accordingly.
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3 Greedy Annealed Pre-Training for a Deep DGA

For the encoder to twist the data into a form that fits the prior $P(H)$, we expect that a very strongly non-linear transformation will be required. As deep autoencoders are notoriously difficult to train (Martens, 2010), adding the extra constraint of making the output of the encoder fit $P(H)$, e.g., factorial, was found experimentally (and without surprise) to be difficult.

What we propose here is to use a an annealing (continuation method) and a greedy pre-training strategy, similar to that previously proposed to train Deep Belief Networks (from a stack of RBMs) (Hinton *et al.*, 2006) or deep autoencoders (from a stack of shallow autoencoders) (Bengio *et al.*, 2007; Hinton and Salakhutdinov, 2006).

3.1 Annealed Training

Since the loss function of Eq.1 is hard to optimize directly, we consider a generalization of the loss function by adding trade-off parameters to the two terms in the loss function corresponding to the reconstruction and prior cost. A zero weight for the prior cost makes the loss function same as that of a standard autoencoder, which is a considerably easier optimization problem.

$$\begin{aligned}\mathcal{L}=&-\beta\sum_i f_i(x)\log P(h_i=1)+(1-f_i(x))\log(1-P(h_i=1))\\&-\sum_j x_j\log P(x_j=1|h=f(x))+(1-x_j)\log(1-P(x_j=1|h=f(x))).\end{aligned} \quad (8)$$

3.1.1 Gradient Descent on Annealed Loss Function

Training DGAs with fixed trade-off parameters is sometimes difficult because it is much easier for gradient descent to perfectly optimize the prior cost by making f map all x to a constant h. This may be a local optimum or a saddle point, escaping from which is difficult by gradient descent. Thus, we use the tradeoff paramters to make the model first learn perfect reconstruction, by setting zero weight for the prior cost. β is then gradually increased to 1. The gradual increasing schedule for β is also important, as any rapid growth in β's value causes the system to 'forget' the reconstruction and prioritize only the prior cost.

A slow schedule thus ensures that the model learns to reconstruct as well as to fit the prior.

3.1.2 Annealing in Deep DGA

Above, we describe the usefulness of annealed training of a shallow DGA. A similar trick is also useful when pretraining a deep DGA. We use different values for these tradeoff parameters to control the degree of difficulty for each pretraining stage. Initial stages have a high weight for reconstruction, and a low weight for prior fitting, while the final stage has β set to unity, giving back the original loss function. Note that the lower-level DGAs can sacrifice on prior fitting, but must make sure that the reconstruction is near-perfect, so that no information is lost. Otherwise, the upper-level DGAs can never recover from that loss, which will show up in the high entropy of $P(x|h)$ (both for the low-level decoder and for the global decoder).

4 Relation to the Variational Autoencoder (VAE) and Reweighted Wake-Sleep (RWS)

The DGA can be seen as a special case of the Variational Autoencoder (VAE), with various versions introduced by Kingma and Welling (2014); Gregor *et al.* (2014); Mnih and Gregor (2014); Rezende *et al.* (2014), and of the Reweighted Wake-Sleep (RWS) algorithm (Bornschein and Bengio, 2014).

The main difference between the DGA and these models is that with the latter the encoder is stochastic, i.e., outputs a sample from an encoding (or approximate inference) distribution $Q(h|x)$ instead of $h = f(x)$. This basically gives rise to a training criterion that is not the log-likelihood but a variational lower bound on it,

$$\log p(x) \geq E_{Q(h|x)}[\log P(h) + \log P(x|h) - \log Q(h|x)]. \tag{9}$$

Besides the fact that h is now sampled, we observe that the training criterion has exactly the same first two terms as the DGA log-likelihood, but it also has an extra term that attempts to maximize the conditional entropy of the encoder output, i.e., encouraging the encoder to introduce noise, to the extent that it does not hurt the two other terms too much. It will hurt them, but it will also help the marginal distribution $Q(H)$ (averaged over the data distribution $Q(X)$) to be closer to the prior $P(H)$, thus encouraging the decoder to contract the "noisy" samples that could equally arise from the injected noise in $Q(h|x)$ or from the broad (generally factorized) $P(H)$ distribution.

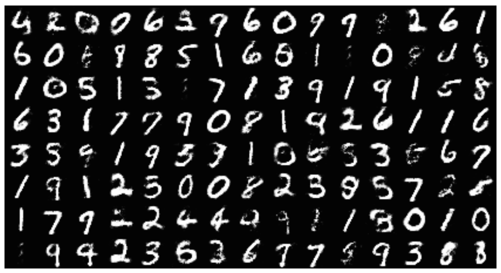
5 Experiments

In this section, we provide empirical evidence for the feasibility of the proposed model, and analyze the influence of various techniques on the performance of the model.

We used the binarized MNIST handwritten digits dataset. We used the same binarized version of MNIST as Murray and Larochelle (2014), and also used the same training-validation-test split.

We trained shallow DGAs with 1, 2 and 3 hidden layers, and deep DGAs composed of 2 and 3 shallow DGAs. The dimension of H was chosen to be 500, as this is considered sufficient for coding binarized MNIST. $P(H)$ is modeled as a factorized Binomial distribution.

Parameters of the model were learnt using minibatch gradient descent, with minibatch size of 100. Learning rates were chosen from 10.0, 1.0, 0.1, and halved whenever the average cost over an epoch increased. We did not use momentum or L1, L2 regularizers. We used tanh activation functions in the hidden layers and sigmoid outputs.


(a)

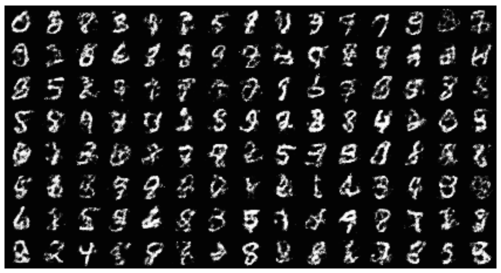

(b)

Figure 3: (a) Samples generated from a 5-layer deep DGA, composed of 3 shallow DGAs of 3 layers (1 hidden layer) each. The model was trained greedily by training the first shallow DGA on the raw data and training each subsequent shallow DGA on the output code of the previous DGA. (b) Sample generated from a 3-layer shallow DGA.

While training, a small salt-and-pepper noise is added to the decoder input to make it robust to inevitable mismatch between the encoder output $f(X)$ and samples from the prior, $h \sim P(H)$. Each bit of decoder input is selected with 1% probability and changed to 0 or 1 randomly.

5.1 Loglikelihood Estimator

When the autoencoder is not perfect, i.e. the encoder and decoder are not perfect inverses of each other, the loglikelihood estimates using Eq. 7 are biased estimates of the true loglikehood. We treat these estimates as an unnormalized probability distribution, where the partition function would be one when the autoencoder is perfectly trained. In practice, we found that the partition function is less than one. Thus, to compute the loglikehood for comparison, we estimate the partition function of the model, which allows us to compute normalized loglikelihood estimates. If $P^*(X)$ is the unnormalized probability distribution, and $\pi(X)$ is another tractable distribution on X from which we can sample, the partition function can be estimated by importance sampling:

$$Z = \sum_x P^*(x) = \sum_x \pi(x) \frac{P^*(x)}{\pi(x)} = E_{x \sim \pi(x)}[\frac{P^*(x)}{\pi(x)}]$$

As proposal distribution $\pi(x)$, We took N expected values $\mu_j = E[X|H_j]$ under the decoder distribution, for $H_j \sim P(H)$, and use them as centroids for a mixture model,

$$\pi(x) = \frac{1}{N} \sum_{j=1}^{N} FactorizedBinomial(x; \mu_j).$$

Therefore,

$$log(P(X)) = log(P^*(X)) - log(Z)$$

gives us the estimated normalized loglikelihood.

5.2 Performance of Shallow vs Deep DGA

The 1-hidden-layer shallow DGA gave a loglikelihood estimate of -118.12 on the test set. The 5-layer deep DGA, composed of two 3-layer shallow DGAs trained greedily, gave a test set loglikelihood estimate of -114.29. We observed that the shallow DGA had better reconstructions than the deep DGA. The deep DGA sacrificed on the reconstructibility, but was more successful in fitting to the factorized Binomial prior.

Qualitatively, we can observe in Figure 3 that samples from the deep DGA are much better than those from the shallow DGA. The samples from the shallow DGA can be described as a mixture of incoherent MNIST features: although all the decoder units have the necessary MNIST features, the output of the encoder does not match well the factorized Binomial of $P(H)$, and so the decoder is not correctly mapping these unusual inputs H from the Binomial prior to data-like samples.

The samples from the deep DGA are of much better quality. However, we can see that some of the samples are non-digits. This is due to the fact that the autoencoder had to sacrifice some reconstructibility to fit H to the prior. The reconstructions also have a small fraction of samples which are non-digits.

5.3 Entropy, Sparsity and Factorizability

We also compared the entropy of the encoder output and the raw data, under a factorized Binomial model. The entropy, reported in Table 1, is measured with the logarithm base 2, so it counts the number of bits necessary to encode the data under the simple factorized Binomial distribution. A lower entropy under the factorized distribution means that fewer independent units are necessary to encode each sample. It means that the probability mass has been moved from a highly complex manifold which is hard to capture under a factorized model and thus requires many dimensions to characterize to a manifold that is aligned with a smaller set of dimensions, as in the cartoon of Figure 2. Practically this happens when many of the hidden units take on a nearly constant value, i.e., the representation becomes extremely "sparse" (there is no explicit preference for 0 or 1 for h_i but one could easily flip the sign of the weights of some h_i in the output layer to make sure that 0 is the frequent value and 1 the rare one). Table 1 also contains a measure of sparsity of the representations based on such a bit flip (so as to make 0 the most frequent value). This flipping allows to count the average number of 1's (of rare bits) necessary to represent each example, in average (third column of the table).

We can see from Table 1 that only one autoencoder is not sufficient to reduce the entropy down to the lowest possible value. Addition of the second autoencoder reduces the entropy by a significant amount.

Since the prior distribution is factorized, the encoder has to map data samples with highly correlated dimensions, to a code with independent dimensions. To measure this, we computed the Frobenius norm of the off-diagonal entries of the correlation matrix of the data represented in its raw form (Data) or at the outputs of the different encoders. See the 3rd columns of Table 1. We see that each autoencoder removes correlations from the data representation, making it easier for a factorized distribution to model.

Samples	Entropy	Avg # active bits	$\|\|Corr - diag(Corr)\|\|_F$
Data (X)	297.6	102.1	63.5
Output of 1^{st} encoder ($f_1(X)$)	56.9	20.1	11.2
Output of 2^{nd} encoder ($f_2(f_1(X))$)	47.6	17.4	9.4

Table 1: Entropy, average number of active bits (the number of rarely active bits, or 1's if 0 is the most frequent bit value, i.e. a measure of non-sparsity) and inter-dimension correlations, decrease as we encode into higher levels of representation, making it easier to model it.

6 Conclusion

We have introduced a novel probabilistic interpretation for autoencoders as generative models, for which the training criterion is similar to that of regularized (e.g. sparse) autoencoders and the sampling procedure is very simple (ancestral sampling, no MCMC). We showed that this training criterin is a lower bound on the likelihood and that the bound becomes tight as the decoder capacity (as an estimator of the conditional probability $P(x|h)$) increases. Furthermore, if the encoder keeps all the information about the input x, then the optimal $P(x|h = f(x))$ is unimodal, i.e., a simple neural network with a factorial output suffices. Our experiments showed that minimizing the proposed criterion yielded good generated samples, and that even better samples could be obtained by pre-training a stack of such autoencoders, so long as the lower ones are constrained to have very low reconstruction error. We also found that a continuation method in which the weight of the prior term is only gradually increased yielded better results.

These experiments are most interesting because they reveal a picture of the representation learning process that is in line with the idea of manifold unfolding and transformation from a complex twisted region of high probability into one that is more regular (factorized) and occupies a much smaller volume (small number of active dimensions). They also help to understand the respective roles of reconstruction error and representation prior in the training criterion and training process of such regularized auto-encoders.

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